

Some Remarks on Multiscale Modeling

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The subject of multiscale modeling is

- ▶ very popular – in many different disciplines,
- ▶ kind of a mess.

Imagine what would happen if we did not have computers before, and all of a sudden, we now have computers and we can solve all the PDEs (and other problems) numerically.

Objective of this talk:

- ▶ A candid assessment of the status of a small part of this vast field.
- ▶ Putting things into perspective
- ▶ Question: What do we need to do in order to turn multiscale modeling into a respectable field of science?

Two types of multiscale problems:

1. Type B: Use microscopic models to bypass ad hoc constitutive modeling.
Example: Non-Newtonian (polymer) fluids – Compute stress from the detailed dynamics of the polymers.
2. Type A: Use microscopic models to resolve singularities (cracks, dislocations, contact lines, reaction zones).

Will focus mostly on Type B problems.

Early examples of multiscale (multi-physics) methods

- ▶ Chemistry: QM-MM (Warshel and Levitt, 1975), Car-Parrinello molecular dynamics (CPMD, 1985)
- ▶ Complex Fluids: Combined kinetic-hydrodynamic models (...)
- ▶ Material Science: CPMD (1985), quasicontinuum methods (Tadmor, Ortiz and Phillips, 1996)

A quick review (for type B problems)

Capturing the macroscale behavior using microscopic models:

- ▶ Car-Parrinello molecular dynamics (CPMD, 1985)
- ▶ Local quasi-continuum method for crystalline solids (Tadmor, Ortiz and Phillips (1996), Knap and Ortiz (2001))
- ▶ Kinetic scheme for gas dynamics (...)

The Car-Parrinello molecular dynamics

- ▶ Macro behavior of interest: Dynamics of the atoms (nuclei)
- ▶ Micro model: Electronic structure models (e.g. density functional theory)
- ▶ Unknown: Force field (don't want to use empirical force field such as Lennard-Jones)
- ▶ “On-the-fly” coupling

Seamless formulation:

Positions of nuclei: $\mathbf{R}_1, \dots, \mathbf{R}_N$

Wavefunctions (orbitals) of electrons: $\phi_1(\cdot), \dots, \phi_M(\cdot)$.

Extended Lagrangian:

$$L\{\mathbf{R}_I, \phi_n, \dot{\mathbf{R}}_I, \dot{\phi}_n\} = \frac{1}{2} \sum_I M_I |\dot{\mathbf{R}}_I|^2 + \frac{1}{2} \sum_n \mu \int \dot{\phi}_n^2(\mathbf{r}) d\mathbf{r} \\ - E_{KS}\{\mathbf{R}_I, \phi_n\} - \sum_{I \neq J} \frac{Z_I Z_J}{|\mathbf{R}_I - \mathbf{R}_J|}$$

where E_{KS} is the energy of the orbitals in Kohn-Sham density functional theory.

How do we choose the parameter μ ?

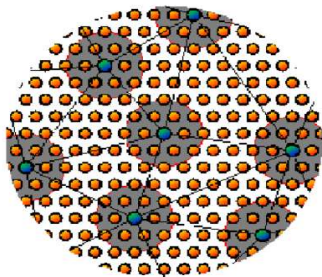
- ▶ Physically, $\mu \sim$ mass of electrons m_e .
- ▶ It determines the fast time scale, hence step size in MD.

Choose μ : $m_e \ll \mu \ll M_I$.

This idea was used in artificial compressibility methods (Chorin).

The local quasicontinuum method

- ▶ Macro behavior of interest: Elastic deformation of crystals
 - ▶ Unknown: Elastic energy functional
 - ▶ Micro model: Atomistic (potential energy in terms of positions of atoms)
1. Select representative atoms and form finite element mesh
 2. Average the potential in a small cluster to obtain at the node.



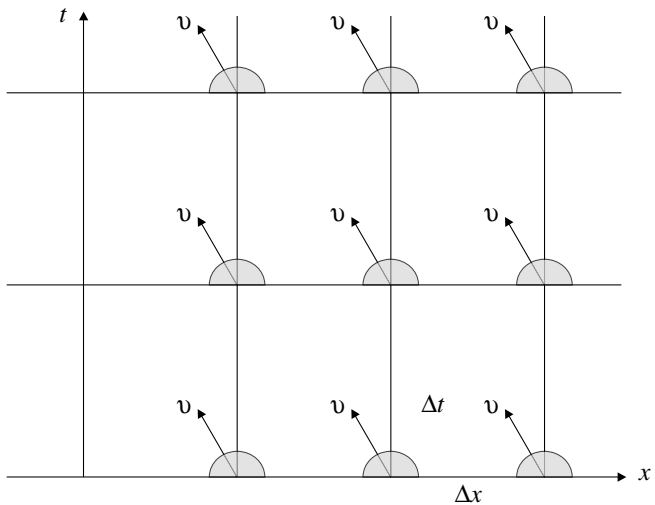
Kinetic schemes for gas dynamics

- ▶ Macro behavior of interest: gas dynamics
- ▶ Unknown: constitutive laws
- ▶ Micro model: kinetic theory

Macro variables $U = (\rho, m, E)$ – density of conserved quantities.

1. Reconstruction: From U^n , find consistent initial condition for the kinetic equation.
2. Solve kinetic equation in neighborhood of cell boundaries.
3. Perform the appropriate averages to find the corresponding fluxes, and use them to find U^{n+1} :

$$U_j^{n+1} = U_j^n - \frac{\Delta t}{\Delta x} (F_{j+1/2}^n - F_{j-1/2}^n)$$



Summary

Common features:

1. Capturing the macroscale behavior using microscopic model/simulation.
2. Making use of scale separation.
 - ▶ Changing the scales of the microscopic system (CPMD).
 - ▶ Solving the microscopic problem locally (local QC and kinetic scheme).

Looking for general strategies

Multiscale, multi-grid method (MMG), A. Brandt (2000).

Traditional multi-grid method: fine scale solver.

But multiscale, multi-grid:

- ▶ Extends the scope of multi-grid method for the purpose of computing only the large scale behavior (not resolving all the small scale details), without the need to obtain a macroscale model first.

“At sufficient coarse level, this entire algorithm effectively produces *macroscopic ‘equations’* for the simulated system This can yield a macroscopic numerical description for the fluid even for those cases where the traditional derivation of closed-form differential equations is inapplicable.”

- ▶ Micro model (KMC, MD, etc) used at the finest level of grids.

- ▶ Linking macro and micro states through “interpolation” and “projection”.
 1. Interpolation: macro to micro
 2. Projection: micro to macro
- ▶ Microscopic model is simulated in *subdomains*, for short times.

“few sweeps are enough, due to the fast CMC equilibration. This fast equilibration also implies that the interpolation can be done just over a restricted *subdomain*, serving as *window*: In the window interior fine-level equilibration is reached.”

These are also the key ideas that motivated HMM and “equation-free”.

But: How do we realize these ideas?

The thesis of Jingrun Chen (The Chinese Academy of Sciences)

Alternative strategies: HMM and 'Equation-free'

HMM (E, Engquist, Vanden-Eijnden, ...)

1. Macroscale solver: Assume a form of macro model, e.g. ODE vs SDE, and then choose a stable numerical scheme for the model.
2. Estimating the missing data: Some data needed in the macro-solver are missing due to the incomplete knowledge of the macro model. These data are estimated from the microscopic model.
 - ▶ The microscopic model should be constrained so that it is consistent with the local macro state of the system.
 - ▶ Analytic expressions are needed to express the needed data in terms of the microscopic solutions.
 - ▶ Special features of the system, such as scale separation, can be exploited to reduce the computational cost. Separation of scales allow us to solve the microscale model on much smaller domains – this is where computational savings come from.

Example: FMM-HMM (J. Huang, ...)

Evaluate

$$\phi(x) = \int_{\Omega} \frac{q(y, \frac{y}{\varepsilon})}{|x - y|} dy$$

where q is a smooth function, periodic in the 2nd variable with period l .

- ▶ Direction application of FMM: Cost = $O(\varepsilon^{-3})$.
- ▶ HMM strategy:
 - ▶ Macro-solver: FMM
 - ▶ Data needed: Coefficients of multipole expansion:

$$M_{k,j}^p = \int_{C_{k,j}} q(y, \frac{y}{\varepsilon})(y - x_{k,j})^p dy$$

where $(C_{k,j}, x_{k,j}) = j$ -th (box, box-center) at k th-level.

$$M_{k,j}^p \simeq \int_{C_{k,j}} \int_l q(y, z)(y - x_{k,j})^p dy dz$$

Example: SDEs

$$\begin{cases} \dot{x} = f(x, y) \\ dy = \frac{1}{\varepsilon} g(x, y) dt + \frac{1}{\sqrt{\varepsilon}} \sigma(x, y) dW(t) \end{cases}$$

Assume macro model in the form: $\dot{x} = F(x)$.

Choose forward Euler as macro solver.

$$\begin{cases} y^{m+1,n} = y^{m,n} + \frac{\delta t}{\varepsilon} g(x^n, y^{m,n}) + \sqrt{\frac{\delta t}{\varepsilon}} w^{m,n}, & m = 0, 1, \dots, M-1 \\ F^n = \frac{1}{M} \sum_{m=1}^M f(x^n, y^{m,n}) \\ x^{n+1} = x^n + \Delta t F^n \end{cases} \quad (1)$$

Successes of HMM

1. A general framework for dealing with many different kinds of multiscale problems:
 - ▶ ODEs and stochastic ODEs
 - ▶ Stochastic simulation algorithms
 - ▶ Homogenization problems
 - ▶ “First-principle-based” constitutive relations for solids and fluids
 - ▶ etc.
2. Links together several existing methods
 - ▶ Local quasicontinuum methods
 - ▶ Kinetic schemes
 - ▶ etc.
3. A nice mathematical framework for analyzing performance of multiscale methods.
4. A natural platform for taking advantage of the special features of the system (scale separation, self-similarity, etc.)

Difficulties with HMM

HMM is quite conservative!

Why assume the form of the macroscale model to begin with? For practical problems, we often know something already about the macroscale model. The form of the macroscale model is often the first kind of questions one would try to answer.

What if we make a wrong assumption about the macroscale model?

Answer: HMM is an 'optimal prediction' strategy: It gives the optimal prediction within the class of models that it considers.

'Equation-free (EF)' (Kevrekidis, Gear, Hyman, ...)

"Enabling microscopic simulators to perform system-level tasks".

A collection of techniques that explicitly take into account scale separation:

1. Coarse bifurcation technique (extension of the Recursive Projection Method (RPM) of Shroff and Keller)
2. Projective integrators (for time)
3. Gap-tooth schemes (for space)
4. Patch dynamics (for time and space)

Example: Projective Integrators

$$\dot{x} = f^\varepsilon(x) = -\frac{1}{\varepsilon}f_0(x) + f_1(x)$$

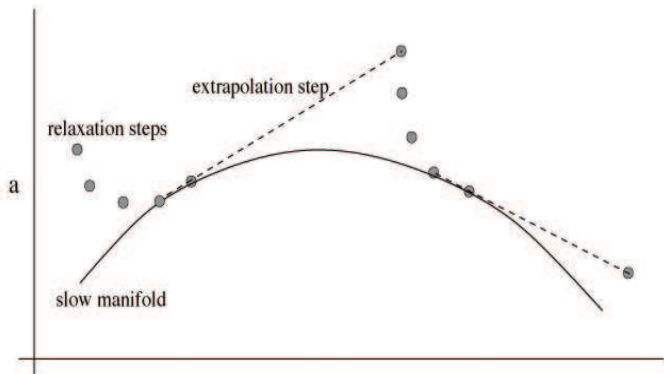
Projective forward Euler:

$$x^{kM+m+1} = x^{kM+m} + \delta t f^\varepsilon(x^{kM+m})$$

$$m = 0, 1, 2, \dots, M - 2,$$

$$x^{kM+1} = x^{kM} + \Delta t f^\varepsilon(x^{kM-1})$$

Similar idea proposed by Ericksson, Johnson and Logg (SISSC, 2003), with different purposes.



Same strategy proposed for MD and SDEs (Hummer and Kevrekidis).

The last step should be viewed as an extrapolation step:

$$\frac{U^{kM+1} - U^{kM}}{\Delta t} = \frac{U^{kM} - U^{kM-1}}{\delta t}$$

where U is (ensemble-averaged) macro variable.

Example: Patch dynamics

- ▶ Lift: From $\{U_j^n\}$, reconstruct initial data for microscopic problem \tilde{u}_0 (e.g. thru interpolation).
- ▶ Evolution: Solve the microscopic model with this initial data \tilde{u}_0 over the small domains (the “teeth”) for some time δt :
 $\tilde{u}_{\delta t} = \mathcal{S}_{\delta t} \tilde{u}_0$.
- ▶ Restriction: Average the microscale solution $\tilde{u}_{\delta t}$ over the small domains, to get $\{\tilde{U}_{\delta t}^n\}$.
- ▶ Extrapolation:

$$U^{n+1} = U^n + \Delta t \frac{\tilde{U}_{\delta t}^n - U^n}{\delta t} \quad (2)$$

or more generally:

$$U^{n+1} = U^n + \Delta t \frac{\tilde{U}_{\delta t}^n - \tilde{U}_{\alpha \delta t}^n}{(1 - \alpha)\delta t} \quad (3)$$

$$0 \leq \alpha < 1$$

Applications:

Micro model:

$$\partial_t u = \partial_x^2 u$$

Initialization: $\tilde{u}_0^j(x) = D_0 + D_1(x - x_j) + \frac{1}{2}D_2(x - x_j)^2,$

$$D_2 = \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{\Delta x^2}, D_1 = \frac{U_{j+1}^n - U_{j-1}^n}{2\Delta x}, D_0 = U_j^n - \frac{1}{24}h^2 D_2$$

This gives

$$U_j^{n+1} = U_j^n + \Delta t D_2$$

Comparison: Similarities

- ▶ Same purpose: All (MMG, HMM, EF) attempt to build a general framework for capturing the macroscale behavior of a system using microscale models, without first deriving or obtaining the macroscale models.
- ▶ Similar basic strategy: Going back and forth between macro and micro states
- ▶ All use scale separation, by limiting the size of the domain or the duration of the microscopic models that have to be simulated.

	Macro to micro	micro to Macro
MMG	interpolation	projection
HMM	reconstruction	compression
Equation-free	lifting	restriction

Differences

- ▶ HMM is macroscale model-based. It starts with an assumption about the form of the macroscale model, and a macroscale solver based on that assumption.
- ▶ 'Equation-free' does not rely on such assumptions (it is much more ambitious). It tries to capture the macroscale behavior by running microscale simulations on small windows and short times,
 - ▶ without making any assumptions about the macroscale model,
 - ▶ without modifying directly the microscale model (so that it applies to legacy codes).
- ▶ Taking advantage of scale separation:
 - ▶ HMM: naturally taken into account in data-estimation step
 - ▶ Equation-free: thru interpolate in space, extrapolate in time.

Driving the legacy codes

This is a very important, practical issue:

- ▶ Common in computational biology and chemistry:
 - ▶ Optimization, control and design
 - ▶ Reaction path analysis
 - ▶ etc.
- ▶ Bifurcation problems: Keller.
- ▶ Optimization problems: Nelder-Mead, etc.

Successes of 'equation-free'

- ▶ Identified and popularized an interesting class of problems:
 - ▶ Coarse bifurcation analysis using microscopic models.
 - ▶ Designing drivers for legacy codes.
- ▶ “Equation-free” is an interesting, ambitious philosophy.
- ▶ Extended the RPM of Schroff and Keller to multiscale bifurcation problems.
- ▶ Projective integrators are extremely simple and also effective for a class of stiff ODEs (think about BGK model).
- ▶

Difficulties with 'equation-free'

- ▶ Applicability of “projective integrators” is limited, e.g. not to SDEs or molecular dynamics.
- ▶ Applicability of “patch dynamics” is limited, e.g. not to convection type of problems.
- ▶ More importantly, the effective macroscale model may be drastically different on different scales.

Conclusion: There are fundamental difficulties with the 'equation-free' philosophy.

Patch dynamics for convection equation

$$\partial_t u + \partial_x u = 0$$

$$U_j^{n+1} = U_j^n + \Delta t(-D_1 + \frac{1}{2}\delta t D_2)$$

Since $\delta t \ll \Delta t$, the last term is much smaller than the other terms, and we are left essentially with

$$U_j^{n+1} = U_j^n - \Delta t D_1$$

What if the macroscale equation is of the form:

$$U_t = U_{xxxx}$$

Then you need to do at least fourth order interpolation.

“Baby-Bathwater” Scheme (Keverkidis et al. 2003)

If the macro model is of the form

$$U_t = F(U, \partial_x U, \partial_x^2 U, \dots, \partial_x^k U)$$

Objective: Find k .

- ▶ Select random numbers $\alpha_0, \alpha_1, \dots, \alpha_k$.
- ▶ Construct initial conditions for microscopic model that are consistent with the macro state U_0 such that $\partial_x^m U_0(0) = \alpha_m$.
- ▶ Use microscopic simulation on a small domain to estimate $U_t(0)$.
- ▶ Test whether $U_t(0)$ depends sensitively on α_k by studying the variance of $U_t(0)$ as a function of α_k .

Difficulties

- ▶ What if we have a macro equation of the form:
$$U_t = U_x + U_{xxxx}?$$
- ▶ The macroscale model depends on the scale we are interested in.
 - ▶ Example: Convection-diffusion in a Benard cell.
 - ▶ Kesten-Papanicolaou

Challenge: How do we overcome these difficulties but still be faithful its original philosophy (e.g. without becoming HMM)?

Givon, D.; Kevrekidis, I. G.; Kupferman, R. Strong Convergence of Projective Integration Schemes for Singularly Perturbed Stochastic Differential Systems. *Comm. Math. Sci.* **4**: 707–729 (2006).

Vanden-Eijnden, E. On HMM-like integrators and projective integration methods for systems with multiple time scales. *Comm. Math. Sci.*, **5**: 495-505 (2007).

More specific issues

- ▶ QM-continuum methods for electronic structure analysis of materials
- ▶ Molecular dynamics simulation of solids with general boundary conditions
- ▶ Incorporating the conformation of polymers into modeling of polymer fluids
- ▶ Influence of molecular interaction in micro-flow
- ▶ etc.

Concluding remarks:

- ▶ Multiscale modeling is the best thing that has happened to applied mathematics in a long time.
- ▶ We have got to be more serious scientifically.